



chain nodes :  
 1 2 3 4 5 6 7 14 15 16 23 24  
 ring nodes :  
 8 9 10 11 12 13 17 18 19 20 21 22 25 26 27 28 29 30  
 chain bonds :  
 1-2 2-3 3-4 3-5 5-6 6-7 7-9 12-14 14-15 14-16 16-17 20-23 23-24 24-27  
 ring bonds :  
 8-9 8-13 9-10 10-11 11-12 12-13 17-18 17-22 18-19 19-20 20-21 21-22 25-26 25-30  
 26-27 27-28 28-29 29-30  
 exact/norm bonds :  
 3-4 3-5 7-9 14-15 14-16 16-17 20-23 23-24 24-27  
 exact bonds :  
 1-2 2-3 5-6 6-7 12-14  
 normalized bonds :  
 8-9 8-13 9-10 10-11 11-12 12-13 17-18 17-22 18-19 19-20 20-21 21-22 25-26 25-30  
 26-27 27-28 28-29 29-30  
  
 Match level :  
 1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom  
 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom  
 22:Atom 23:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom